Benzoic acid, 3,6-dichloro-2-hydroxy-3401-80-7 | DTXSID9041657

3401-80-7	DTXSID9041657	

Model Performance

Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 4.53

Global applicability domain: Inside

Local applicability domain index: 4.02e-01

Confidence level: 7.12e-01

Nearest Neighbors from the Training Set

Image not found

Dalapon-sodium Measured: 7.24 Predicted: 5.61

Image not found

2-Chlorobenzoic acid Measured: 10.0 Predicted: 3.89

Image not found

Trichloroacetic acid Measured: 1.70 Predicted: 2.22

Image not found

Phenylphosphinic acid Measured: 6.03 Predicted: 4.42

Image not found

2,2-Dimethylpropanoic acid

Measured: 2.29 Predicted: 2.74